New Numerical Method for Fermion Field Theory

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Abstract

A new deterministic, numerical method to solve fermion field theories is presented. This approach is based on finding solutions Z[J] to the lattice functional equations for field theories in the presence of an external source J. Using Grassmann polynomial expansions for the generating functional Z, we calculate propagators for systems of interacting fermions. These calculations are straightforward to perform and are executed rapidly compared to Monte Carlo. The bulk of the computation involves a single matrix inversion. Because it is not based on a statistical technique, it does not have many of the difficulties often encountered when simulating fermions. Since no determinant is ever calculated, solutions to problems with dynamical fermions are handled more easily. This approach is very flexible, and can be taylored to specific problems based on convenience and computational constraints. We present simple examples to illustrate the method; more general schemes are desirable for more complicated systems.

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1 Introduction

The need for new calculational probes of quantum field theory is well-known. Despite the success of various iterative methods including perturbation theory, many problems, especially for strongly coupled systems, persist in both high energy and condensed matter physics. The advent of high performance computers has made numerical attacks on these problems practical. Most of these approaches have roots in Monte Carlo methods. They form the basis of many calculations in statistical mechanics, including nonrelativistic field theory, and have been co-opted by high energy physics for lattice gauge theory calculations [1].

In high energy physics, Monte Carlo methods had remarkable initial successes in calculating various quantities associated with quantum field theory. Unfortunately, even for simple systems, calculations involving dynamical fermions, or performed on large lattices, become expensive in both time and computer resources. Despite refined algorithms and enormous increases in computer power, progress with Monte Carlo based methods has been slow compared to the initial impressive successes. For lattice QCD [2], detailed studies of systems with dynamical quarks with low masses may require computer time well beyond current capabilities.

In condensed matter physics, understanding models of strongly correlated electrons using numerical methods has serious limitations. Much of this work has been based on exact diagonalization or quantum Monte Carlo. Diagonalization is powerful especially for calculating dynamical properties, but in practice, is limited to small systems. Typically, 4x4 clusters are the largest that can be studied. Alternatively, Monte Carlo methods can examine larger lattices, but for fermionic systems, simulations face serious problems. This includes the so-called "minus sign" problem which makes defining a positive-definite probability measure problematic [11]. This difficulty plagues many models, including many of those relevant to high T_c superconductivity.

We have formulated a numerical scheme for lattice quantum field theory which does not rely on any statistical method and is not restricted to small systems [3, 4, 5, 6]. This approach is based on considering QFT in the presence of an external source. Using either the operator equations of motion, or equivalently the path integral representation, equations can be derived for the vacuum persistence amplitude Z. On a lattice, the result is a set of coupled *linear* differential equations for Z in the discretized sources. For fermionic problems, these sources will be anticommuting Grassmann variables. Once we have obtained Z, the lattice Green's functions can be extracted by functional differentiation.

Despite the large number of coupled differential equations for Z, one for each source variable, there is nothing unusual about this problem mathematically. We can solve them as we do any set of linear differential equations. Since at the end of any calculation the sources are set to zero, the obvious first choice is to expand Z in a power series in the sources about the origin. For fermionic systems with only a few sites, exact solutions for Z are possible. This is due to the self-terminating nature of Grassmann polynomials. In general, we cannot solve the theory exactly, and therefore, we must introduce an approximation. For the purposes of this paper, we truncate the series expansion for Z after some maximum power in the source variables. In this way, we obtain a closed, finite set of linear equations for the expansion coefficients accurate to within the limits of the approximation.

The coupled differential equations have a high degree of symmetry due to the translation and reflection invariance of the underlying periodic lattice. This structure can be used to great advantage in constructing solutions, greatly reducing the number of equations to be considered. This reduced set of algebraic equations for the coefficients of Z is necessarily inconsistent; this being an artifact of the approximation. There are many ways to deal with this problem. One particularly elegant method is to require that weighted averages of the truncated equations vanish. A clever choice of weight functions speeds the convergence of the truncated equations to the exact solution. Numerical techniques of this sort are called Galerkin methods and are well-known [8].

Since our expansion and weight functions depend on the external sources, we call this method "the Source Galerkin method" [3]. It is different in concept and application from any other technique that we know of for solving quantum field theory. As a practical matter, fermions and bosons are treated in a similar manner. Consequently, solutions for dynamical fermion problems may be possible with existing computers. On the other hand, this method is not without difficulties. Principally, the power series grows quickly, making

examination of large systems difficult. In these cases, different basis functions must be used. The examples presented here illustrate one of the simpler formulations, but not generally the most useful.

This paper is organized as follows. Section Two gives a general overview of the bosonic formulation of the Source Galerkin method. Section Three outlines the Source Galerkin formulation for fermions. The functional formulation is identical to the boson case except that the sources become anticommuting Grassmann variables. The partition function Z satisfies a set of coupled Grassmann differential equations. As with bosons, we solve these equations by power series in the source variables. In Section Four, we examine small lattice systems where exact solutions are possible. For more realistic systems, the series must be truncated and a Galerkin procedure devised. We propose a Galerkin method for fermions in Section Five and perform calculations on 1D self-interacting fermion systems. We close by illustrating the flexibility of the Source Galerkin method with respect to the choice of expansion functions. We study 2D lattice Gross-Neveu model by examining the leading behavior of Z as $J \to 0$. The first term is equivalent to a Gaussian. We calculate the behavior of the chiral condensate as an order parameter for chiral symmetry breaking. A method to calculate corrections is outlined.

2 Source Galerkin Method

In this section, we review the bosonic formulation of the Source Galerkin method. We study quantum field theory in the presence of an external source. The vacuum persistence amplitude $Z[J] =_J \langle 0|0\rangle_J$ is the generating functional for the Green's functions. It is constrained by a functional differential equation. For a self-interacting scalar field theory, the dynamics are described by

$$L_J(\phi) = 1/2\,\hat{\phi}\,(\Box + M^2)\,\hat{\phi} + g/4\,\hat{\phi}^4 + J\hat{\phi}.\tag{1}$$

Taking vacuum expectation values of the operator equations of motion

$$(\Box + M^2)\langle \hat{\phi} \rangle_J + g \langle \hat{\phi}^3 \rangle_J = J_J \langle 0 | 0 \rangle_J \tag{2}$$

and identifying Euclidean expectation values of fields with functional derivatives of Z[J]

$$G(x_1 \dots x_n) = \frac{\delta^n Z[J]}{\delta J(x_1) \dots \delta J(x_n)}$$
(3)

yields the functional relation

$$(\Box + M^2) \frac{\delta Z}{\delta J(x)} + g \frac{\delta^3 Z}{\delta J(x)^3} = J Z. \tag{4}$$

After solving this equation for Z, we can extract all information about our field theory by functional differentiation. On a D-dimensional Euclidean lattice, the functional equation becomes a set of coupled differential equations

$$(2D + M^2)\frac{\partial Z}{\partial J(i)} - \sum_{nn} \frac{\partial Z}{\partial J(i)} + g\frac{\partial^3 Z}{\partial J(i)^3} = J(i)Z$$
 (5)

where the sum is over nearest neighbors. There is one equation per site.

For finite lattices with N sites, Z as a multivariate function of the N source variables J(i). To construct a solution to the differential equations, we can expand Z on any complete set of functions in the source variables

$$Z = \sum_{n} a_n \, \phi_n(\{J\}) \tag{6}$$

where a_n are the unknowns of the problem. A particularly simple choice is polynomial functions. It should be emphasized that other choices are preferred for more complicated systems. We consider this possibility in Section Seven.

The number of independent unknown coefficients can be reduced by exploiting the symmetries of the lattice. For polynomial expansions, Z can be constructed to be invariant under the symmetry group of the lattice

$$Z = \sum_{n,m} a_{n,m} P_{n,m} \tag{7}$$

where $P_{n,m}$ are invariant polynomials in the source variables of order n and with m invariant classes for a given order. The coefficients $a_{n,m}$ are to be determined. The number of invariant classes for a given order depends on both the number of lattice sites and on the number of symmetry operations for a given lattice. For example, higher dimensional lattices have larger symmetry groups and therefore have fewer independent unknowns. These polynomials form a lattice invariant basis upon which we can construct solutions for Z.

In order to solve the differential equations, we must specify boundary conditions. Normalization of the vacuum amplitude implies

$$Z[J=0] = 1 \tag{8}$$

and we exclude symmetry breaking

$$\frac{dZ}{dJ(i)}|_{J=0} = \langle \phi(i) \rangle = 0. \tag{9}$$

We cannot specify the second derivatives of Z because they correspond to the two-point functions. Instead, w truncate Z at some finite order M. The truncation order is dictated by computational constraints. As a boundary condition, truncation guarantees that as $g \to 0$ in the interaction theory, the solution reduces to the free field. This is possible only for path integral formulations constrained to real integration contours [5, 7, 9]. Truncation in this sense not only sets a boundary condition, but also introduces an approximation scheme. This scheme is made systematic by truncating at successively higher orders, and then taking the limit as M goes to infinity.

We fit our trial solution to the differential equations using the Galerkin method. The truncated polynomial is an approximate solution to the differential equations where the error due to truncation is called the residual R [8]. In order to minimize R, we define an inner product in the source space

$$(g,f) = \int_{-\epsilon}^{\epsilon} g(J(1)\dots J(N))f(J(1)\dots J(N))[dJ]$$
(10)

where the integration is over all J(i), and ϵ is considered small. Requiring the inner product of R with linearly independent test functions T_k to vanish

$$(R, T_1) = 0$$

$$\vdots$$

$$(R, T_i) = 0$$

$$(11)$$

generates a set of linear algebraic equations. We can generate as many of these equations as we like as long as the T_k are linearly independent.

In analogy with a variational principle, we chose the test functions as

$$T_k = \frac{d}{dJ(1)} P_{n,m} \tag{12}$$

where the $P_{n,m}$ are the invariant polynomial that formed the basis for Z_T . This choice guarantees that we always have as many equations as unknowns, and experience has shown that it gives rapid convergence of Z_T to the exact solution. We construct as many equations as there are independent unknowns in our power series solution These equations can be solved by a single matrix inversion where the resulting coefficients are the lattice Green's functions.

3 Fermion Formulation

We now construct the lattice functional equations for fermions. As with the bosonic case, we appeal to a generating function Z to calculate the consequences of our fermionic field theory. We begin by considering a 1D system of spinless free fermions in the presence of external sources. We will see that the inclusion of interactions requires only minor modifications. Our system has dynamics described by the following action

$$S = \sum_{i=1}^{N} \frac{1}{2} \bar{\psi}(i) [\psi(i+1) - \psi(i-1)] + M\bar{\psi}(i)\psi(i) + [\bar{\eta}(i)\psi(i) + \bar{\psi}(i)\eta(i)]. \tag{13}$$

where the sum runs over an N site lattice and periodic boundary conditions are assumed. Grassmann sources $\bar{\eta}(i), \eta(i)$ live on each site of the lattice and are coupled to the fields. Taking the variation of the action with respect to the fields, we obtain the EOM for the field operators $\psi(i)$

$$\frac{1}{2}[\psi(i+1) - \psi(i-1)] + M\psi(i) + \eta(i) = 0.$$
(14)

There are analogous equations for the conjugates. Taking vacuum matrix elements of this equation, and identifying expectation values of fields with Grassmann Source derivatives of the generating functional $Z[\bar{\eta}, \eta]$.

$$\frac{\partial Z}{\partial \eta(i)} = \langle \bar{\psi}(n) \rangle \qquad \frac{\partial Z}{\partial \bar{\eta}(n)} = -\langle \psi(n) \rangle, \tag{15}$$

gives the lattice equations for Z.

$$\frac{1}{2} \left[\frac{\partial Z}{\partial \bar{\eta}(i+1)} - \frac{\partial Z}{\partial \bar{\eta}(i-1)} \right] + M \frac{\partial Z}{\partial \bar{\eta}(i)} - \eta(i) Z = 0.$$
 (16)

As with the boson case, there is one equation (and its conjugate) for each site of the lattice. Our fermion field theory is completely specified by this set of coupled Grassmann PDEs for Z plus boundary conditions. The Green's functions can be calculated as derivatives of $Z[\bar{\eta}, \eta]$ about $\bar{\eta}, \eta = 0$.

We solve these equations with a Grassmann power series

$$Z = \sum_{n_i, \bar{n}_i = 0.1} a_{\bar{n}_1, n_1 \cdots \bar{n}_N, n_N} \bar{\eta}(1)^{n_1} \cdots \bar{\eta}(N)^{n_N} \eta(1)^{n_1} \cdots \eta(N)^{n_N}.$$
(17)

Because of Fermi statistics, Z is at most linear in each source variable. This means that for finite systems, the power series terminates at a finite order independent of any approximation such as truncation. Therefore, exact solutions exist for finite series. To reduce the number of independent coefficients in this series, we take advantage of symmetries of the system. In addition to the space-time symmetries, the Action conserves fermion number

$$\psi(i) \to e^{i\theta} \psi(i)$$

and is invariant under charge conjugation

$$\psi(i) \to -\bar{\psi}(i) \quad \bar{\psi}(i) \to \psi(i).$$

For bipartite lattices, we have the additional symmetries

$$\psi(i) \to -\psi(i)$$
 if $i = odd$

$$\psi(i) \to \psi(i)$$
 if $i = even$.

We construct the terms in our series explicitly to reflect all these symmetries.

4 Exact Solutions for Four Site Model

To be specific, consider a free fermion field on four sites. We place complex spinless fields and sources on each site. This gives eight coupled Grassmann differential equations for Z including the conjugate equations. Since they are all related by symmetry operations, it is sufficient to use only one equation to constrain our solution as long as Z is constructed explicitly to reflects these symmetries. We choose

$$\frac{1}{2} \left[\frac{\partial Z}{\partial \bar{\eta}(2)} - \frac{\partial Z}{\partial \bar{\eta}(4)} \right] + M \frac{\partial Z}{\partial \bar{\eta}(1)} - \eta(1) Z = 0.$$
 (18)

With four complex sources in our system, there are eight independent degrees of freedom. Since Z can be at most linear in each Grassmann variable, the polynomial expansion can be at most eighth order. All higher terms vanish due to statistics. Therefore for four sites, we can find an exact solution with only an eighth order Grassmann series. This polynomial has 69 terms which can be grouped into 14 independent symmetry classes. For example, at second order we have

$$Z = 1 + a_1 \left[\bar{\eta}(1)\eta(1) + \bar{\eta}(2)\eta(2) + \bar{\eta}(3)\eta(3) + \bar{\eta}(4)\eta(4) \right]$$

$$+ a_2 \left[\bar{\eta}(2)\eta(1) + \bar{\eta}(3)\eta(2) + \bar{\eta}(4)\eta(3) + \bar{\eta}(1)\eta(4) \right]$$

$$- \bar{\eta}(1)\eta(2) - \bar{\eta}(2)\eta(3) - \bar{\eta}(3)\eta(4) - \bar{\eta}(4)\eta(1) \right]$$

$$+ a_3 \left[\bar{\eta}(3)\eta(1) + \bar{\eta}(4)\eta(2) + \bar{\eta}(1)\eta(3) + \bar{\eta}(2)\eta(4) \right]$$
(19)

where the coefficients are the Green's functions

$$a_{1} = \langle \bar{\psi}(1)\psi(1)\rangle$$

$$a_{2} = \langle \bar{\psi}(2)\psi(1)\rangle$$

$$a_{3} = \langle \bar{\psi}(3)\psi(1)\rangle$$
(20)

Since this is an exact solution, no Galerkin procedure is needed. We can apply the Grassmann equation to the full polynomial, set all the coefficients of the resulting power series to zero, and solve the resulting system of equations. For the exact solution, we have as many independent equations as unknowns and our set of algebraic equations for the coefficients of Z is completely specified. The result for the free two-point function is

$$a_{1} = \frac{2M^{2} + 1}{2M(M^{2} + 1)}$$

$$a_{2} = \frac{1}{2(M^{2} + 1)}$$

$$a_{3} = \frac{1}{2M(M^{2} + 1)}$$
(21)

The complete results for all the Green's functions can be found in the Appendix. These results agree identically with these from inverting the propagator matrix, or equivalently from the lattice Fourier transformed solution to the Green's function equation.

We can generalize our action to include self-interactions

$$S = \sum_{i}^{N} \frac{1}{2} \bar{\psi}(i) [\psi(i+1) - \psi(i-1)] + M \bar{\psi}(i) \psi(i)$$

$$+ \frac{G}{2} \bar{\psi}(i) \psi(i) [\bar{\psi}(i+1) \psi(i+1) + \bar{\psi}(i-1) \psi(i-1)]$$

$$+ [\bar{\eta}(i) \psi(i) + \bar{\psi}(i) \eta(i)].$$
(22)

In terms of the lattice functional equations, this means adding third order derivative terms to the differential equations

$$-\frac{G}{2}\frac{\delta^3 Z}{\delta \bar{\eta}(i)\delta \eta(i+1)\delta \bar{\eta}(i+1)} - \frac{G}{2}\frac{\delta^3 Z}{\delta \bar{\eta}(i)\delta \eta(i-1)\delta \bar{\eta}(i-1)}$$
(23)

We solve the interacting model just as we did for the free case. Again, we find an exact solution yielding the following coefficients

$$a_{1} = \frac{2M^{3} + (2G+1)M}{2M^{4} + (4G+2)M^{2} + G^{2} + G}$$

$$a_{2} = \frac{2M^{2} + G}{4M^{4} + (8G+4)M^{2} + 2G^{2} + 2G}$$

$$a_{3} = \frac{M}{2M^{4} + (4G+2)M^{2} + G^{2} + G}$$
(24)

Notice that the coefficients respect the free field limit as $g \to 0$, and therefore correspond to the path integral solution.

5 Galerkin Method for Fermions

For larger lattices, even though the power series is self-terminating, it becomes too unwieldy for practical calculations. Therefore, we truncate the exact expansion at some lower order, and determine the coefficients numerically. As in the boson case, we have the problem of inconsistent equations. While the series expansion for Z contains the full symmetry group of the Action, the individual Grassmann differential operators are invariant under only a subgroup. The algebraic relations for the coefficients of the truncated Z are therefore overdetermined. This implies that an approximate procedure is needed to determine the coefficients.

The Galerkin procedure is based on an attempt to minimize the error function, or the residual R, about the origin in source space

$$R = \hat{D}_i^F Z_T[\bar{\eta}, \eta] \tag{25}$$

where \hat{D}_i^F is the fermionic source operator centered at site i and $Z_T[\bar{\eta}, \eta]$ is the truncated partition function that depends on the Grassmann sources $\bar{\eta}, \eta$. The residual represents the error induced by truncation. For bosons, in order to minimize the error, we defined an inner product in the space spanned by functions of the source variables $\{J(1), \ldots, J(N)\}$.

$$(g, f) = \int_{-\epsilon}^{\epsilon} \dots \int_{-\epsilon}^{\epsilon} g(J(1) \dots J(N)) f(J(1) \dots J(N)) dJ(1) \dots dJ(N)$$
 (26)

We demand that inner products of R with linearly independent test functions $\{T_j\}$ vanish, and solved the resulting algebraic equations. In this way, we have fitted our approximation to a solution of the differential equation. Solutions obtained in the manner are called "weak solutions" where convergence is guaranteed in the mean.

As a first attempt to mimic this procedure for fermions, we could begin by defining an inner product in the Grassmann function space [10]. Unfortunately, there are several problems with this approach. Principally, taking a Grassmann inner product of R with Grassmann test functions is a very severe operation. In fact, the Grassmann inner product kills off most of the equations that we want to solve. Furthermore, recall that for bosons, the Galerkin method gave average solutions in an ϵ -neighborhood of the origin; they represented "weak" solutions to the differential equations. Since Grassmann integration is really a formal construct with no measure theoretic interpretation, then in what sense are they average solutions?

Instead, we propose to sidestep all these difficulties by making a few simple observations. First of all, the Grassmann sources which create all of the difficulties carry virtually no physics. All the information about a QFT is contained in the coefficients of Z, i.e. the Green's functions, which are simple real numbers. The sources are arbitrary, and in fact, for fermionic problems, their only real role is to give the correct signs in the Green's functions equations for the coefficients. Once we have obtained R, all the physical information has been completely specified. Any manipulations of R which are mathematically consistent does not alter the physics.

With these observations in mind, we propose the following alternative Galerkin method for fermions. Once we have R, we relax the anticommutivity of all source variables, and allow them to be integrated in the usual way, using the boson inner product. Test functions are constructed as derivatives of scalar polynomials that have the same symmetry as the fermion invariant polynomials. The rest of the calculation proceeds identically as for the boson case; inner products of R with scalar test functions gives algebraic relations for the coefficients of Z. After solving this system of equations, ϵ is taken to zero.

A more compact way to view this procedure is to consider each source variable as being decomposed into a scalar piece times a Grassmann unit vector

$$\eta(i) = \mu \,\hat{\eta}(i). \tag{27}$$

The unit vector $\hat{\eta}(i)$ carries the anticommutivity and enforces the commutation relations while μ acts like a length that can be integrated in the usual sense. In this framework, the functional equations act on the Grassmann piece while the Galerkin inner product operates on the scalar component.

6 Numerical Solutions

We test our truncation/Galerkin procedure against the four site model discussed previously. Since we can solve this system exactly, it is useful for checking the convergence of our method. Solutions for this model were found using an eighth order Grassmann polynomial. To examine the convergence of our method, we first truncate this series at fourth order. Since this is not an exact solution, we use a Galerkin approach to find an approximate one. The expressions for the coefficients are complicated rational functions of the parameters. Setting M = 1.0, the results are

$$a_{1} = \frac{2117446 G + 7294107}{1786968 G^{2} + 9742031 G + 9725476}$$

$$a_{2} = \frac{3092325 G + 4862738}{2(1786968 G^{2} + 9742031 G + 9725476)}$$

$$a_{3} = \frac{330478 G + 2431369}{1786968 G^{2} + 9742031 G + 9725476}$$
(28)

g	4th Order	6th Order	Exact
0	0.75	0.75	0.75
0.1	0.7003	0.7089	0.7095
0.5	0.5553	0.5840	0.5926
1.0	0.4428	0.4803	0.5
10	0.0996	0.1160	0.1494

Table 1: Convergence of fermionic Galerkin method for $\langle \bar{\psi}(1)\psi(1)\rangle$

g	4th Order	6th Order	Exact
0	0.25	0.25	0.25
0.1	0.2413	0.2334	0.2328
0.5	0.2130	0.1928	0.1852
1.0	0.1871	0.1677	0.15
10	0.0626	0.1141	0.0390

Table 2: Convergence of fermionic Galerkin method for $\langle \bar{\psi}(2)\psi(1)\rangle$

These should be compared against the exact solution in Eq (6.78). Similarly, we truncate at sixth order, finding

$$a_{1} = \frac{3(618904 G + 510825)}{1345887 G^{2} + 3667541 G + 2043300}$$

$$a_{2} = \frac{(G+2)(278354 G + 510825)}{2(1345887 G^{2} + 3667541 G + 2043300)}$$

$$a_{3} = \frac{278354 G + 510825}{1345887 G^{2} + 3667541 G + 2043300}$$
(29)

To see exactly how these answers converge, we substitute a range of values for G and examine the behavior of the coefficients. Results for the two-point functions are displayed in the tables.

For large lattices, we need to perform calculations numerically. We calculated the interacting propagator for an eight site lattice in one dimension. Results are presented for a Grassmann polynomial truncated at fourth and sixth order. These are nontrivial calcula-

g	4th Order	6th Order	Exact
0	0.25	0.25	0.25
0.1	0.2299	0.2223	0.2217
0.5	0.1726	0.1543	0.1481
1.0	0.1299	0.1118	0.1
10	0.0201	0.0190	0.0065

Table 3: Convergence of fermionic Galerkin method for $\langle \bar{\psi}(3)\psi(1)\rangle$

tions since the fourth order polynomial alone has 124 coefficients. These coefficients must be determined by the Galerkin method.

The results are checked against a mean field calculation. In general, mean field theory is not exact, but represents only a single pole approximation to the propagator. Our propagator, on the other hand, should include contributions from all poles. Thus, only loose comparisons should be made between the mean field results and the Source Galerkin numbers.

It should be noted that calculations with the Source Galerkin method are very efficient, especially when compared to Monte Carlo. Typically, for lattice gauge theory, the fermions must be quenched to make calculations tractable. Here, determination of the interacting propagator for a system of dynamical fermions presents no special difficulty. The bulk of a calculation involves a single matrix inversion for a given set of parameters. This is in contrast to Monte Carlo where many sweeps through the lattice are necessary to reduce statistical error. As the plots show, the Source Galerkin calculations are very clean. They show rapid convergence compared to the mean field results even at intermediate couplings and using only low order polynomials.

4th Order	6th Order	Mean Field
0.5458	0.5831	0.6287
0.2288	0.2104	0.2218
0.0883	0.0753	0.0797
0.0177	0.0329	0.0243
0.0166	0.0267	0.0196

Table 4: Interacting Propagator on 8 Sites with M=1.0, g=0.5

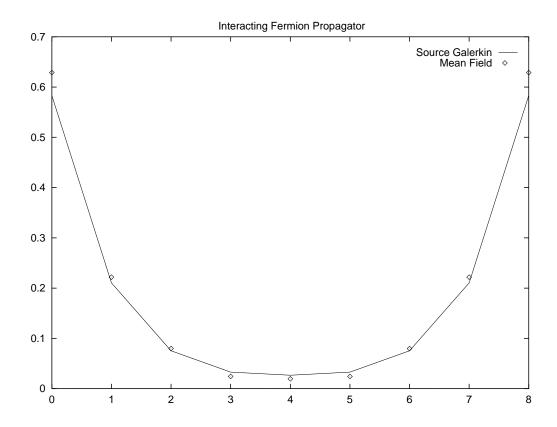


Figure 1: 8 site lattice with M=1.0 and G=0.5

7 Leading Behavior of the Gross-Neveu Model

Since the computational complexity grows rapidly with the number of sites, we need to go beyond simple polynomial expansions to examine larger systems. It is important to note that we are not restricted to power series expansion. Any complete set of functions is allowed where the choice is restricted only by convenience. We exploit this flexibility with respect to the choice of expansion functions. A more general choice is a Gaussian ansatz. This choice leaves only one unknown parameter to solve, independent of the lattice size. We will use this ansatz to examine the structure of a nontrivial model of interacting relativistic fermions.

The Gross-Neveu model [12] is a (1+1)-dimensional renormalizable field theory of N species of Dirac fermions interacting through a 4-fermion term. The action is given by

$$L = \sum_{j=1}^{N} \left[\psi^{\bar{j}} \partial_j \psi^{(j)} - \frac{1}{2} g^2 (\psi^{\bar{j}}) \psi^{(j)} \right]^2$$
 (30)

where the four-fermion term is often replaced by a quadratic term with the help of a real scalar field σ

$$L = \sum_{j=1}^{N} \left[\psi^{\bar{j}} \partial \psi^{(j)} + \frac{1}{2g^2} \sigma^2 + \sigma \psi^{\bar{j}} \psi^{(j)} \right]. \tag{31}$$

The action displays a discrete chiral symmetry

$$\psi \rightarrow \gamma_5 \psi$$

$$\bar{\psi} \rightarrow -\bar{\psi} \gamma_5$$

$$\sigma \rightarrow -\sigma$$

where $\gamma_5 = i \gamma_1 \gamma_2$. The model can be studied analytically by the saddle point method, leading to a 1/N expansion for $g^2 N$ fixed. At leading order, the chiral condensate is given by

$$\langle \sigma \rangle = \Lambda e^{-\pi/(g^2 N)}.$$
 (32)

The theory describes a free fermion where the dynamical mass $m_f = \langle \sigma \rangle$ results from spontaneous chiral symmetry breaking.

We apply the Source Galerkin method to this model. For simplicity, we employ staggered fermions. To probe the details of the system, we need lattices considerably larger than the ones used in the 1D example. For such lattices, construction and manipulation of the Grassmann invariant polynomials becomes difficult. Instead, we take advantage of the extreme flexibility of the Galerkin method with regards to the choice of expansion functions. Following a similar calculation for scalar ϕ^4 [5], we determine the leading asymptotic behavior for vanishing sources $J \to 0$ of the GNM.

After including sources $(\bar{\eta}_n, \eta_n, S_n)$ for the fermion and auxiliary fields, we vary the staggered GN action to obtain the equations of motion

$$(D_{n,m} + \sigma_n) \chi_n^{\alpha} = \eta_n^{\alpha}$$

$$\frac{\sigma_n}{2\lambda} + \sum_{n=1}^{\alpha} \bar{\chi}_n^{\alpha} \chi_n^{\alpha} = S_n$$
(33)

where

$$D_{n,m} = \frac{1}{2} \left[\delta_{n,m+\hat{1}} - \delta_{n,m-\hat{1}} \right] + \frac{1}{2} \left(- \right)^{n_1} \left[\delta_{n,m+\hat{2}} - \delta_{n,m-\hat{2}} \right]$$
(34)

is the Susskind differential operator with $\hat{1},\hat{2}$ being unit vectors along the two Euclidean directions and where $\lambda=g^2N$. After taking matrix elements and inserting functional definitions, we obtain the lattice functional equations

$$D_{n,m} \frac{\delta Z}{\delta \bar{\eta}_n^{\alpha}} + \frac{\delta^2 Z}{\delta S_n \delta \bar{\eta}_n^{\alpha}} = \eta_n^{\alpha} Z$$

$$\frac{1}{2\lambda} \frac{\delta Z}{\delta S_n} + \sum_{n=1}^{\alpha} \frac{\delta^2 Z}{\delta \bar{\eta}_n^{\alpha} \delta \eta_n^{\alpha}} = S_n Z$$
(35)

We solve these equations with a Gaussian in the sources

$$Z = e^{W(\bar{\eta}, \eta)} \tag{36}$$

and find the following equations for $W(\bar{\eta}, \eta)$

$$[D_{n,m} + \frac{\delta W}{\delta S_n}] \frac{\delta Z}{\delta \bar{\eta}_n^{\alpha}} = \eta_n^{\alpha}$$

$$\frac{N}{2\lambda} \frac{\delta W}{\delta S^n} + \sum_{n=1}^{\alpha} \left[\frac{\delta^2 W}{\delta \bar{\eta}_n^{\alpha} \delta \eta_n^{\alpha}} + (\frac{\delta W}{\delta \bar{\eta}_n^{\alpha}}) (\frac{\delta W}{\delta \eta_n^{\alpha}}) \right] = S_n.$$
(37)

Expanding W in a 2nd order power series in the Grassmann sources gives

$$W(\bar{\eta}, \eta) = \bar{\eta}_k G(k - j)\eta_j \tag{38}$$

where G(k-j) is the interacting propagator. Since σ_n is not dynamical, we ignore it at this order, and set $\delta W/\delta S$ which measures chiral symmetry breaking equal to a constant

$$\frac{\delta W}{\delta S} = \langle \, \sigma \, \rangle = \sigma_0. \tag{39}$$

Keeping only linear terms in the sources, we obtain a dynamical equation

$$[D_{n,m} + \sigma_0] G(n-m) = \delta_{n,m}$$

$$\tag{40}$$

as well as a constraint equation.

$$\frac{N}{\lambda} = G(0). \tag{41}$$

The dynamical equation suggests that G(n-m) has the form of a free staggered propagator with mass σ_0 . We can solve this equation by Fourier transform

$$G(n-m) = \frac{1}{L^2} \sum_{p_1=0}^{L-1} \sum_{p_2=0}^{L-1} \frac{\sigma_0 + i \sin(p_1) + i(-)^{m_1} \sin(p_2)}{\sigma_0^2 + \sin^2(p_1) + \sin^2(p_2)} e^{ip(n-m)}$$
(42)

where n, m, p are two dimensional vectors. Putting this expression into the constraint gives a gap equation for σ_0 that must be solved self-consistently

$$\frac{1}{\lambda} = \frac{1}{L^2} \sum_{p_1=0}^{L-1} \sum_{p_2=0}^{L-1} \frac{1}{\sigma_0^2 + \sin^2(p_1) + \sin^2(p_2)}.$$
 (43)

This type of equation is familiar from large N expansions.

It is important to note that this solution has been obtained by fitting a Gaussian

$$Z = \exp \omega(\bar{\eta}, \eta) \tag{44}$$

to the functional equations where we kept only second order terms in the expansion for W

$$\omega(\bar{\eta}, \eta) = \bar{\eta}_i G_{i,k} \eta_k + \dots \tag{45}$$

At this level of approximation, the procedure may seem rather trivial. The results we have obtained are closely related to the usual large N expansion results. However, it should be noted that our numerical procedure has determined the leading order solution of a nontrivial fermionic problem. Systematic improvements of approximations are then possible where the Gaussian is only the leading contribution. By considering Z as a Gaussian multiplied by a power series, it is possible to improve our leading order result. The Galerkin method can be used to determine the coefficients of the polynomials.

8 Conclusion

We have presented a new numerical method to solve lattice fermion theories. It is based on the differential formulation of QFT in the presence of an external source. By examining the functional differential equations for a theory on a finite lattice, we obtained a set of coupled Grassmann PDEs for the generating functional Z. For nonlinear field theories with polynomial interactions, these equations are always linear. Once Z is obtained, the lattice Green's functions can be extracted by functional differentiation.

To construct solutions, we can expand Z on any complete set of functions in the source variables $\{\eta_i\}$. A particularly simple choice is polynomial functions. We saw that these functions gave very rapid convergence even using low order polynomials. Calculations were efficient to perform and produced very clean numbers. The bulk of any calculation involved only a single matrix inversion. The matrix to be inverted becomes large, but unlike Monte Carlo, there is only one inversion for a given set of parameters.

Due to computational complexity, polynomial basis functions are limited to small lattices. For larger systems, more general schemes are possible. The Galerkin procedure of fitting approximate solutions to the functional equations allows tremendous freedom in choosing expansion functions. We illustrated one possibility by using a Gaussian to extract the leading behavior of the solution. In this formulation, we had only one unknown parameter, independent of the size of the lattice. Systematic corrections can then be calculated. We will have more to say about other generalized approaches in future communications.

This method is deterministic, and therefore, does not suffer from many of the problems usually associated with numerical solutions of fermionic problems. For example, Monte Carlo simulations of lattice gauge theories have difficulty including dynamical fermions. But with the Source Galerkin method, calculation of the interacting propagator presents no special complication. In addition, fermionic systems at nonzero chemical potential have problems defining a positive definite probability measure for simulations due to the "minus sign" problem. Since our method is deterministic, this is not an issue.

9 Appendix A: Exact Coefficients for Four Site Model

$$A1 = \frac{2\,M^2 + (2\,G + 1)\,M}{2\,M^4 + (4\,G + 2)\,M^2 + G^2 + G}$$

$$A2 = \frac{2 M^2 G}{2 M^4 + (4 G + 2) M^2 + G^2 + G}$$

$$A3 = \frac{M}{2 M^4 + (4 G + 2) M^2 + G^2 + G}$$

$$A4 = \frac{4 M^2 + 2 G + 1}{4 M^4 + (8 G + 4) M^2 + 2 G^2 + 2 G}$$

$$A5 = \frac{M}{2M^4 + (4G + 2)M^2 + G^2 + G}$$

$$A6 = \frac{1}{4 M^4 + (8 G + 4) M^2 + 2 G^2 + 2 G}$$

$$A7 = \frac{M}{2M^4 + (4G + 2)M^2 + G^2 + G}$$

$$A8 = \frac{1}{4M^4 + (8G+4)M^2 + 2G^2 + 2G}$$

$$A9 = \frac{2 M^2}{2 M^4 + (4 G + 2) M^2 + G^2 + G}$$

$$A10 = 0$$

$$A11 = \frac{2M}{2M^4 + (4G+2)M^2 + G^2 + G}$$

$$A12 \ = \ \frac{1}{2\,M^4 + (4\,G + 2)\,M^2 + G^2 + G}$$

$$A13 = 0$$

$$A14 = \frac{2}{2M^4 + (4G+2)M^2 + G^2 + G}$$

10 Appendix B: Fourth Order Coefficients with M=1.0

$$A1 = \frac{2117446\,G + 7294107}{1786968\,G^2 + 9742031\,G + 9725476}$$

$$A2 = \frac{3092325\,G + 4862738}{2(1786968\,G^2 + 9742031\,G + 9725476)}$$

$$A3 = \frac{330478\,G + 2431369}{1786968\,G^2 + 9742031\,G + 9725476}$$

$$A4 = \frac{3573936 G + 12156845}{2(1786968 G^2 + 9742031 G + 9725476)}$$

$$A5 \ = \ \frac{792533\,G + 2431369}{1786968\,G^2 + 9742031\,G + 9725476}$$

$$A6 \ = \ \frac{2431369}{2(1786968\,G^2 + 9742031\,G + 9725476)}$$

$$A7 = \frac{792533 G + 2431369}{1786968 G^2 + 9742031 G + 9725476}$$

$$A8 = -\frac{736530\,G - 2431369}{2(1786968\,G^2 + 9742031\,G + 9725476)}$$

$$A9 = \frac{1061159\,G + 4862738}{1786968\,G^2 + 9742031\,G + 9725476}$$

$$A10 = \frac{24642 \, G}{1786968 \, G^2 + 9742031 \, G + 9725476}$$

11 Appendix C: Sixth Order Coefficients with M=1.0

$$A1 = \frac{3(618904 G + 510825)}{1345887 G^2 + 3667541 G + 2043300}$$

$$A2 = \frac{(G+2)(278354\,G + 510825)}{2(1345887\,G^2 + 3667541\,G + 2043300)}$$

$$A3 = \frac{278354 G + 510825}{1345887 G^2 + 3667541 G + 2043300}$$

$$A4 = \frac{5(482684 \, G + 510825)}{2(1345887 \, G^2 + 3667541 \, G + 2043300)}$$

$$A5 = \frac{278354 G + 510825}{1345887 G^2 + 3667541 G + 2043300}$$

$$A6 = \frac{278354 G + 510825}{2(1345887 G^2 + 3667541 G + 2043300)}$$

$$A7 = \frac{278354 \, G + 510825}{1345887 \, G^2 + 3667541 \, G + 2043300}$$

$$A8 = \frac{278354 G + 510825}{2(1345887 G^2 + 3667541 G + 2043300)}$$

$$A9 = \frac{2(278354\,G + 510825)}{1345887\,G^2 + 3667541\,G + 2043300}$$

$$A10 = 0$$

$$A11 = \frac{1021650}{1345887 G^2 + 3667541 G + 2043300}$$

$$A12 = \frac{510825}{1345887 G^2 + 3667541 G + 2043300}$$

$$A13 = \frac{556708\,G}{1345887\,G^2 + 3667541\,G + 2043300}$$

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